

Gerd B Rocha

List of Publications by Year in descending order

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70
papers

2,465
citations

304602

22
h-index

206029

48
g-index

70
all docs

70
docs citations

70
times ranked

2679
citing authors

#	ARTICLE	IF	CITATIONS
1	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. <i>Journal of Computational Chemistry</i> , 2006, 27, 1101-1111.	1.5	634
2	GPU Linear Algebra Libraries and GPGPU Programming for Accelerating MOPAC Semiempirical Quantum Chemistry Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3072-3081.	2.3	222
3	NAMD goes quantum: an integrative suite for hybrid simulations. <i>Nature Methods</i> , 2018, 15, 351-354.	9.0	149
4	Sparkle Model for the Calculation of Lanthanide Complexes: AM1 Parameters for Eu(III), Gd(III), and Tb(III). <i>Inorganic Chemistry</i> , 2005, 44, 3299-3310.	1.9	133
5	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3333-3341.	2.3	107
6	Repurposing approved drugs as inhibitors of SARS-CoV-2 S-protein from molecular modeling and virtual screening. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 3924-3933.	2.0	102
7	Sparkle Model for AM1 Calculation of Lanthanide Complexes: Improved Parameters for Europium. <i>Inorganic Chemistry</i> , 2004, 43, 2346-2354.	1.9	65
8	Sparkle/PM3 for the modeling of europium(III), gadolinium(III), and terbium(III) complexes. <i>Journal of the Brazilian Chemical Society</i> , 2009, 20, 1638-1645.	0.6	59
9	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. <i>RSC Advances</i> , 2013, 3, 16747.	1.7	58
10	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. <i>Journal of Molecular Modeling</i> , 2006, 12, 373-389.	0.8	56
11	Synthesis and Luminescent Properties of Novel Europium(III) Heterocyclic β^2 -Diketone Complexes with Lewis Bases: Structural Analysis Using the Sparkle/AM1 Model. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4129-4137.	1.0	47
12	On the charge factors of the simple overlap model for the ligand field in lanthanide coordination compounds. <i>Chemical Physics Letters</i> , 2000, 331, 519-525.	1.2	43
13	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 64-74.	2.3	37
14	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). <i>Chemical Physics Letters</i> , 2006, 425, 138-141.	1.2	36
15	RM1 Model for the Prediction of Geometries of Complexes of the Trications of Eu, Gd, and Tb. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3031-3037.	2.3	36
16	On the use of combinatory chemistry to the design of new luminescent Eu ³⁺ complexes. <i>Chemical Physics Letters</i> , 2005, 405, 123-126.	1.2	35
17	Efficacy of the semiempirical sparkle model as compared to ECP ab-initio calculations for the prediction of ligand field parameters of europium (III) complexes. <i>Journal of Luminescence</i> , 2005, 111, 81-87.	1.5	32
18	Synthesis and conformational study of a new class of highly bioactive compounds. <i>Chemical Physics Letters</i> , 2007, 449, 336-340.	1.2	31

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19	Design of ligands to obtain lanthanide ion complexes displaying high quantum efficiencies of luminescence using the sparkle model. <i>Computational and Theoretical Chemistry</i> , 2000, 527, 245-251.	1.5	30
20	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5897-5900.	1.1	28
21	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1588-1596.	2.3	27
22	Efficient synthesis of 16 aromatic Morita-Baylis-Hillman adducts: Biological evaluation on <i>Leishmania amazonensis</i> and <i>Leishmania chagasi</i> . <i>Bioorganic Chemistry</i> , 2010, 38, 279-284.	2.0	25
23	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 177, 225-237.	2.0	23
24	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes: Sparkle/PM3. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5015-5018.	1.1	23
25	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2584-2588.	0.8	22
26	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). <i>Journal of Organometallic Chemistry</i> , 2008, 693, 1952-1956.	0.8	22
27	3-Hydroxy-2-methylene-3-(4-nitrophenyl)propanenitrile: A new highly active compound against epimastigote and trypomastigote form of <i>Trypanosoma cruzi</i> . <i>Bioorganic Chemistry</i> , 2010, 38, 190-195.	2.0	21
28	Revisiting the origin of the preferential π - π stacking conformation of the (+)-8-phenylmenthyl acrylate. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 1718-1726.	0.6	19
29	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). <i>Journal of Computational Chemistry</i> , 2005, 26, 1524-1528.	1.5	18
30	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). <i>Chemical Physics Letters</i> , 2007, 441, 354-357.	1.2	18
31	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 4099-4102.	0.8	17
32	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). <i>Chemical Physics Letters</i> , 2005, 411, 61-65.	1.2	17
33	1,3-thiazolium-5-thiolates mesoionic compounds: semiempirical evaluation of their first static hyperpolarizabilities and synthesis of new examples. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 934-940.	0.6	17
34	Elucidating Enzymatic Catalysis Using Fast Quantum Chemical Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 578-591.	2.5	17
35	Sparkle/AM1 modeling of holmium (III) complexes. <i>Polyhedron</i> , 2005, 24, 3046-3051.	1.0	15
36	Sparkle model for the AM1 calculation of dysprosium (III) complexes. <i>Inorganic Chemistry Communication</i> , 2005, 8, 831-835.	1.8	15

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37	Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives. <i>Journal of Molecular Structure</i> , 2021, 1244, 131224.	1.8	13
38	Cerium (III) Complexes Modeling with Sparkle/PM3. <i>Lecture Notes in Computer Science</i> , 2007, , 312-318.	1.0	13
39	Reverse saturable absorption and anti-Stokes fluorescence in mesoionic compounds pumped at 532 nm. <i>Applied Optics</i> , 2001, 40, 1389.	2.1	12
40	A DFT and Natural Resonance Theory investigation of the electronic structure of mesoionic compounds. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	12
41	Semiempirical methods do Fukui functions: Unlocking a modeling framework for biosystems. <i>Journal of Computational Chemistry</i> , 2020, 41, 862-873.	1.5	12
42	Theoretical nonlinear optics equivalence between mesoionic and polyenic bridges in push-pull compounds. <i>Journal of the Brazilian Chemical Society</i> , 2005, 16, 583-588.	0.6	11
43	DFT/PCM, QTAIM, 1H NMR conformational studies and QSAR modeling of thirty-two anti-Leishmania amazonensis Morita's Baylis-Hillman Adducts. <i>Journal of Molecular Structure</i> , 2012, 1022, 72-80.	1.8	11
44	Sparse Projected-Gradient Method As a Linear-Scaling Low-Memory Alternative to Diagonalization in Self-Consistent Field Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1043-1051.	2.3	11
45	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. <i>PLoS ONE</i> , 2014, 9, e86376.	1.1	10
46	Determining the Relative Binding Affinity of Ricin Toxin A Inhibitors by Using Molecular Docking and Nonequilibrium Work. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1205-1213.	2.5	10
47	Assessment of semiempirical enthalpy of formation in solution as an effective energy function to discriminate native-like structures in protein decoy sets. <i>Journal of Computational Chemistry</i> , 2016, 37, 1962-1972.	1.5	9
48	Theoretical characterization of the shikimate 5-dehydrogenase reaction from Mycobacterium tuberculosis by hybrid QC/MM simulations and quantum chemical descriptors. <i>Journal of Molecular Modeling</i> , 2020, 26, 297.	0.8	7
49	A higher flexibility at the SARS-CoV-2 main protease active site compared to SARS-CoV and its potentialities for new inhibitor virtual screening targeting multi-conformers. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 9214-9234.	2.0	7
50	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. <i>Journal of the Brazilian Chemical Society</i> , 2018, , .	0.6	6
51	Synthesis, spectroscopic characterization, DFT studies, and preliminary antimicrobial evaluation of new antimony(III) and bismuth(III) complexes derived from 1,3,5-triazine. <i>Journal of Molecular Structure</i> , 2019, 1183, 373-383.	1.8	6
52	PRIMoRDIA: A Software to Explore Reactivity and Electronic Structure in Large Biomolecules. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5885-5890.	2.5	6
53	GPU algorithms for density matrix methods on MOPAC: linear scaling electronic structure calculations for large molecular systems. <i>Journal of Molecular Modeling</i> , 2020, 26, 313.	0.8	6
54	Thermochemical and Quantum Descriptor Calculations for Gaining Insight into Ricin Toxin A (RTA) Inhibitors. <i>ACS Omega</i> , 2021, 6, 8764-8777.	1.6	6

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55	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. <i>Chemical Physics Letters</i> , 2006, 420, 230-234.	1.2	5
56	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. <i>PLoS ONE</i> , 2015, 10, e0124372.	1.1	5
57	Would the solvent effect be the main cause of band shift in the theoretical absorption spectrum of large lanthanide complexes?. <i>Journal of Molecular Structure</i> , 2011, 997, 30-36.	1.8	4
58	A topological assessment of the electronic structure of mesoionic compounds. <i>Journal of Computational Chemistry</i> , 2015, 36, 1907-1918.	1.5	4
59	Synthesis, thermochemical and quantum chemical studies on antimony(III) and bismuth(III) complexes with 2,2'-bipyridine and 1,10-phenanthroline. <i>Thermochimica Acta</i> , 2019, 676, 234-240.	1.2	4
60	Discovery of RTA ricin subunit inhibitors: a computational study using PM7 quantum chemical method and steered molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 5427-5445.	2.0	4
61	Synthesis, characterization and spectroscopic study of Eu(III) complexes with 3-aminopicolinic acid derivatives. <i>Journal of Luminescence</i> , 2005, 113, 79-88.	1.5	3
62	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. <i>PLoS ONE</i> , 2016, 11, e0154500.	1.1	3
63	Performance assessment of semiempirical molecular orbital methods in the structural prediction of Sb(III) and Bi(III) complexes. <i>Journal of Molecular Modeling</i> , 2013, 19, 4575-4584.	0.8	2
64	RM1 modeling of neodymium, promethium, and samarium coordination compounds. <i>RSC Advances</i> , 2015, 5, 12403-12408.	1.7	2
65	Spin states of Mn(III) meso-tetraphenylporphyrin chloride assessed by density functional methods. <i>Journal of Molecular Modeling</i> , 2017, 23, 363.	0.8	2
66	Efficient algorithm for expanding theoretical electron densities in cartesian zernike functions. <i>Journal of Computational Chemistry</i> , 2018, 39, 2022-2032.	1.5	2
67	Synthesis, in silico Study, Theoretical Stereochemistry Elucidation and Antifungal Activity of New Imides Derived from Safrole. <i>Journal of the Brazilian Chemical Society</i> , 0, , .	0.6	1
68	Synthesis, Spectroscopic Characterization, DFT Calculations and Preliminary Antifungal Activity of New Piperine Derivatives. <i>Journal of the Brazilian Chemical Society</i> , 0, , .	0.6	0
69	A Simple Strategy That Uses Molecular Dynamics and Semiempirical Methods for the Conformational Searching of isomers of the Macrocyclic Complex Na[Gd(DOTA)·H ₂ O]. <i>Revista Virtual De Quimica</i> , 0, , 641-655.	0.1	0
70	Investigation of the structural dynamics of a knotted protein and its unknotted analog using molecular dynamics. <i>Journal of Molecular Modeling</i> , 2022, 28, 108.	0.8	0